12 Oct 2024

# SC Quantathon v1 (Team 1)
# Xanadu Challenge: Spectral gap for molecules

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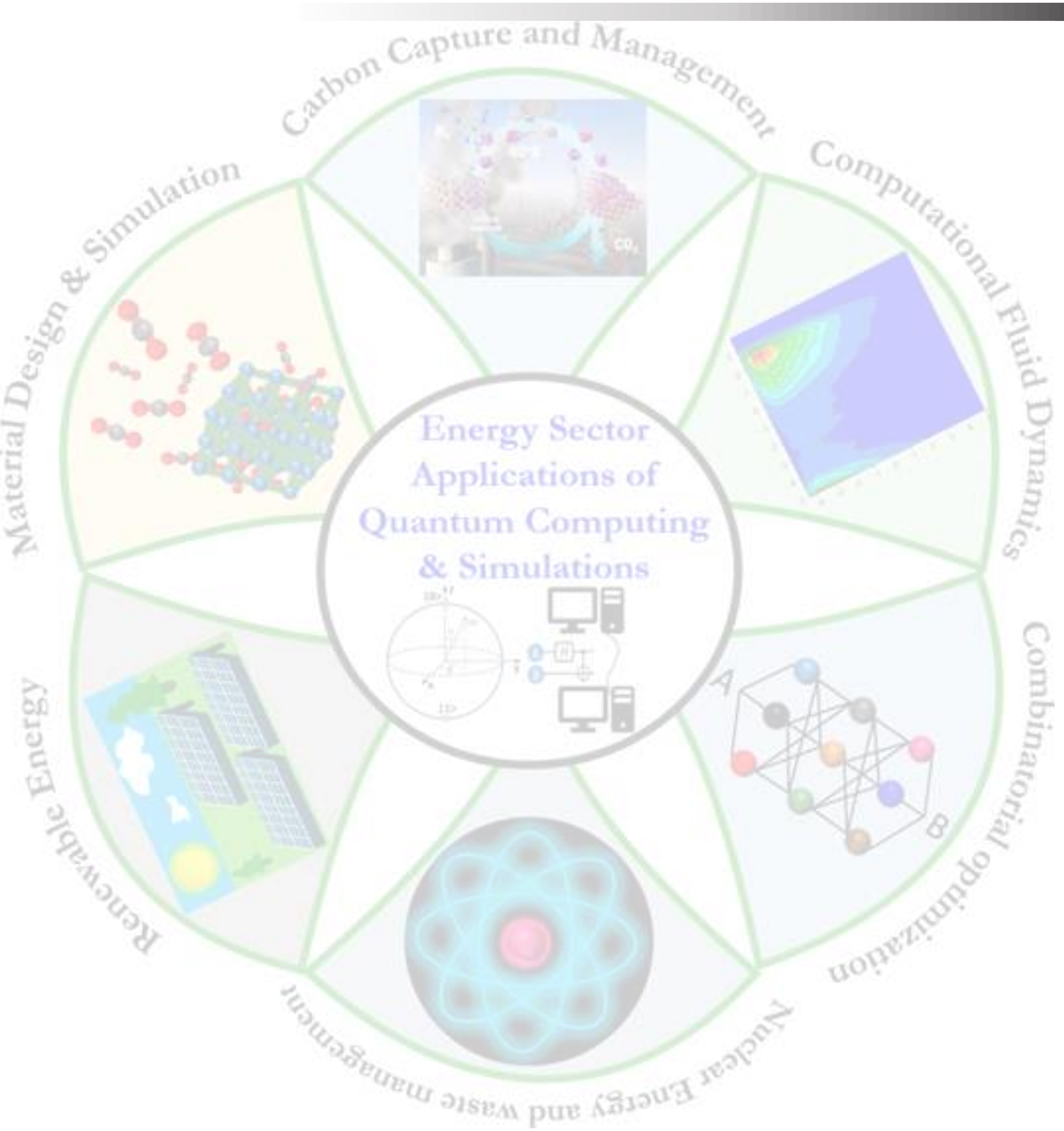
North Carolina State University

# Motivation


Carbon Capture and Management
Computational Fluid Dynamics
Combinatorial Optimization
Nuclear Energy and waste management
Renewable Energy
Material Design & Simulation
Energy Sector Applications of Quantum Computing & Simulations

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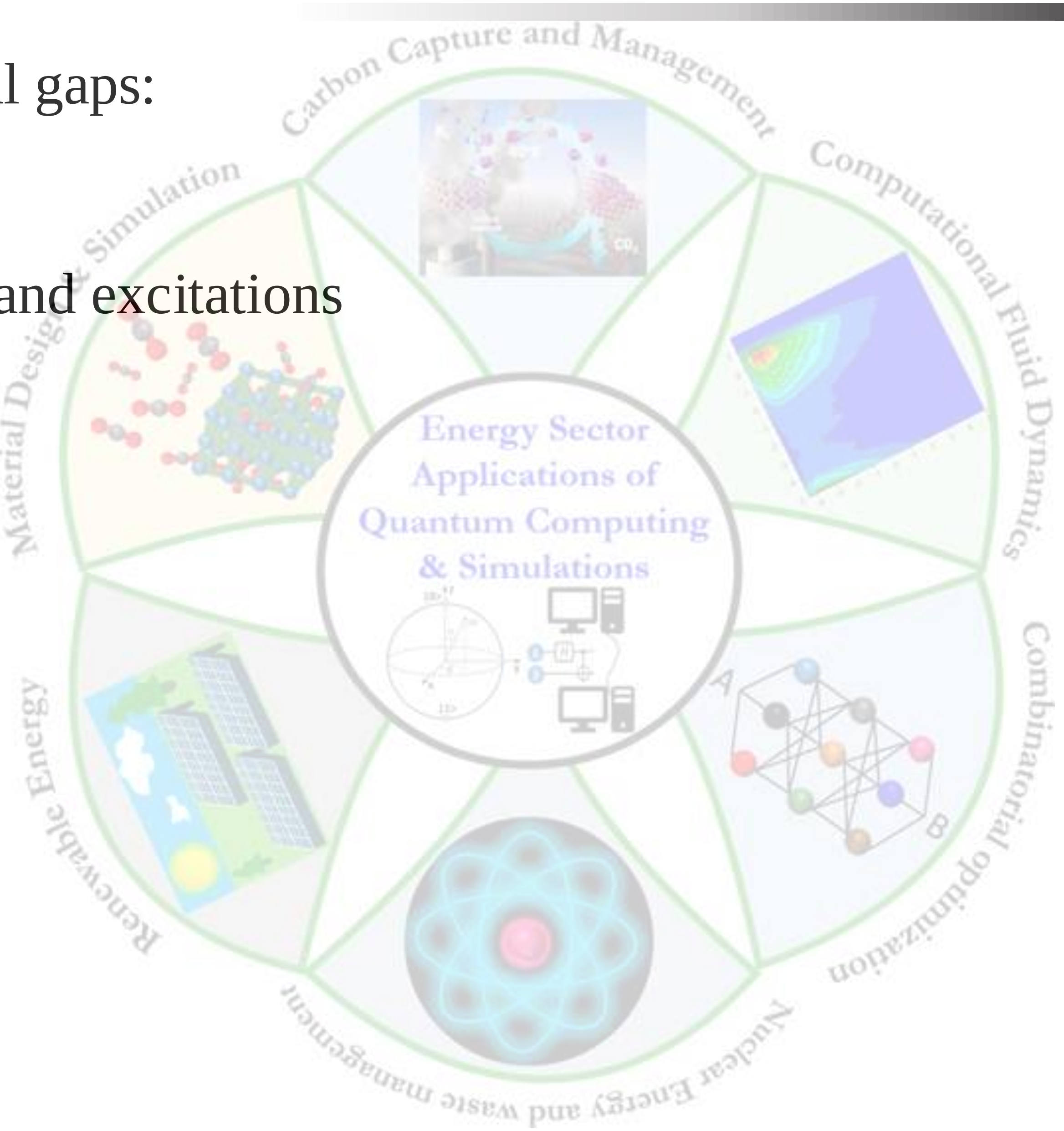
Importance of spectral gaps:

- Stability
- Reactivity
- Photo-interactions and excitations
- Material properties
- Algorithm designs



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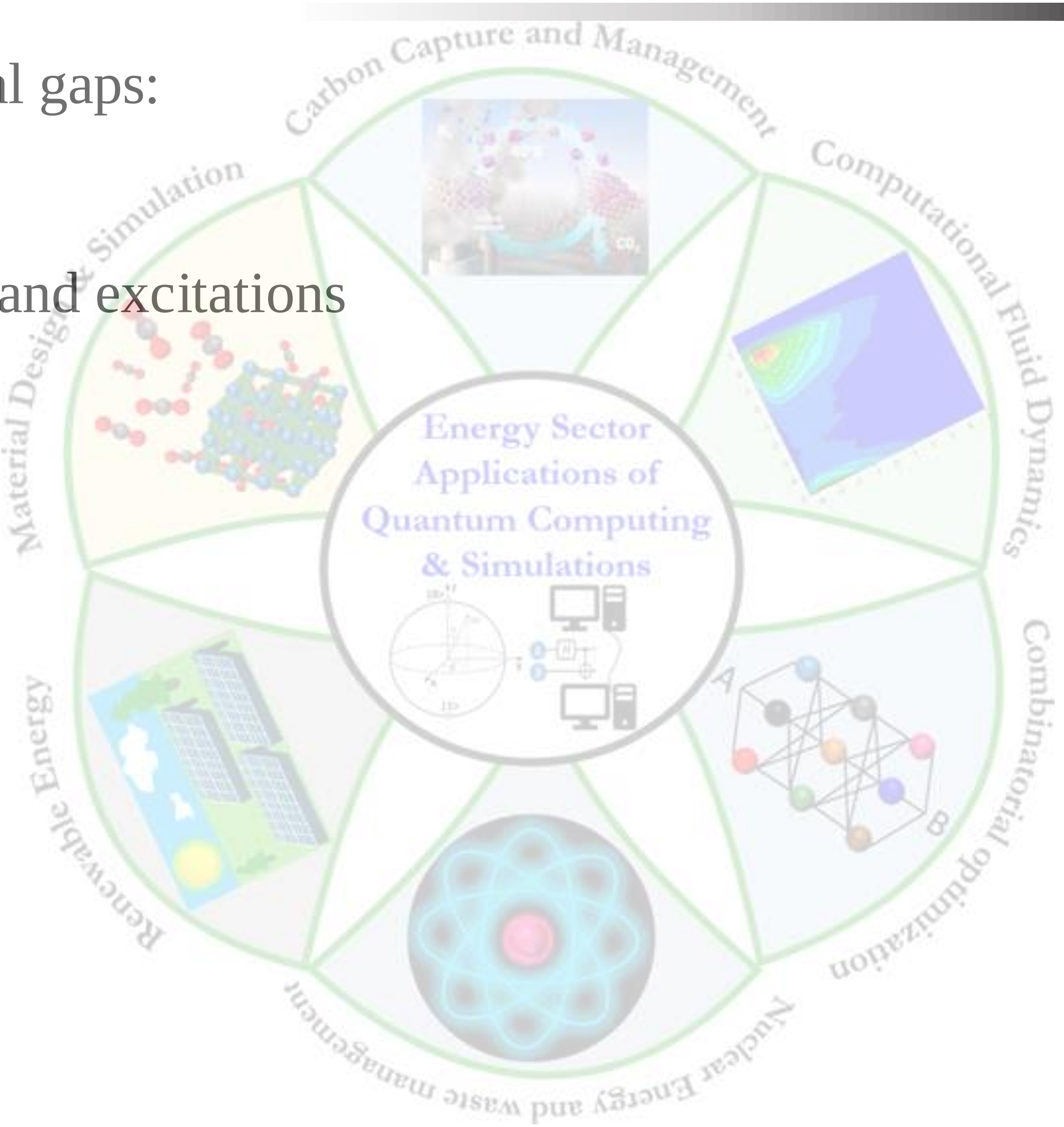

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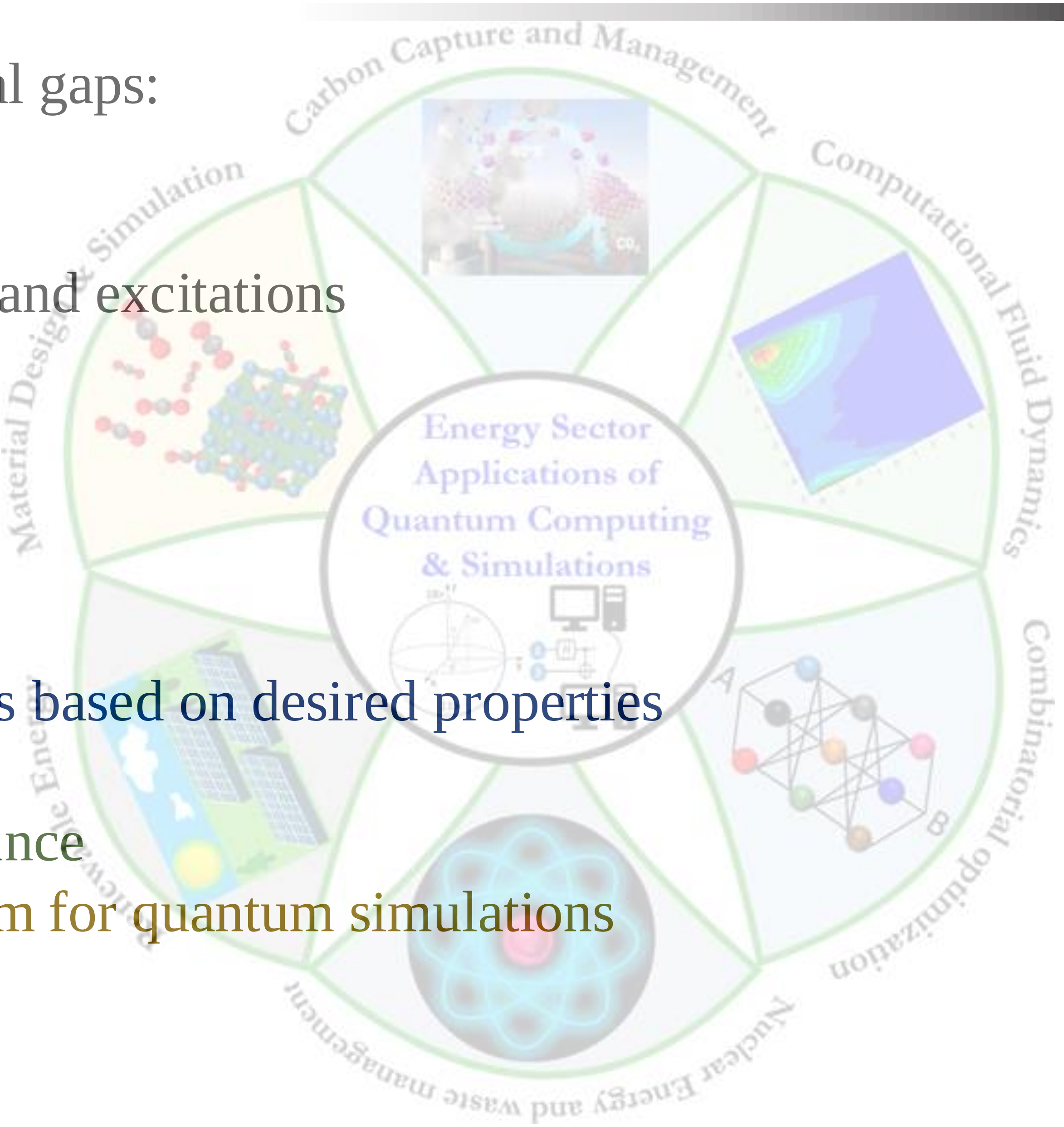
Applications:
1. Choosing materials based on desired properties (Material search)
2. Experiment assistance
3. Choice of algorithm for quantum simulations
4. Material design



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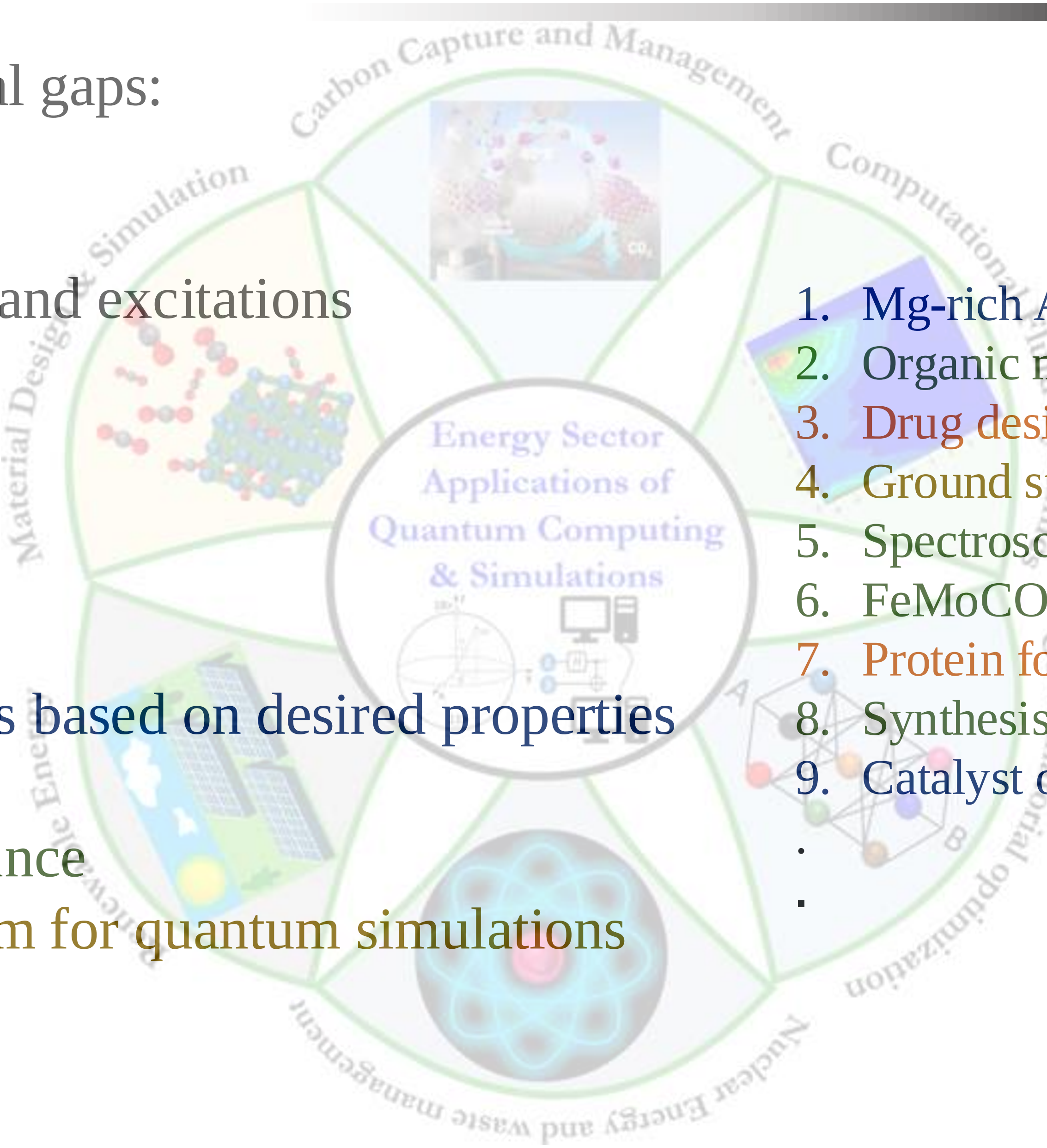


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1. Mg-rich Anticorrosive Coating Design
2. Organic molecules combustion energy
3. Drug design
4. Ground state energy estimation
5. Spectroscopy experiments
6. FeMoCO
7. Protein folding
8. Synthesis of cyclic ozone (Fuel tech)
9. Catalyst optimization and fabrication

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# Our chosen path

## Application choice: Metallification of H2 molecule

- Variation of bond length impacts the properties of the molecule (Insulator-semiconductor-metal)
- Experiments are designed to get different phases by changing the bond length
- Bond length changes the spectral gaps and hence the reaction properties

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Get the energy spectrum as a function of bond length

SD + EC

→

Choose an optimal bond length

Min Eigenvalue

→

Get the spectral gap

Linear response

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# Eigenvector continuation as a subspace method

$\mathcal{H}_{target}(\theta) = \{H(\theta_1), H(\theta_2), \dots H(\theta_n)\}$

Choose $k_p$ points in θ space

θ - Bond length

$\{H(\theta_1), H(\theta_2), \dots H(\theta_{k_p})\}$

*Use any (truncated) state preparation method to solve for (approximate) ground state*

$\{|\phi_1\rangle, |\phi_2\rangle, \dots |\phi_{k_p}\rangle\}$

*Low-energy subspace*

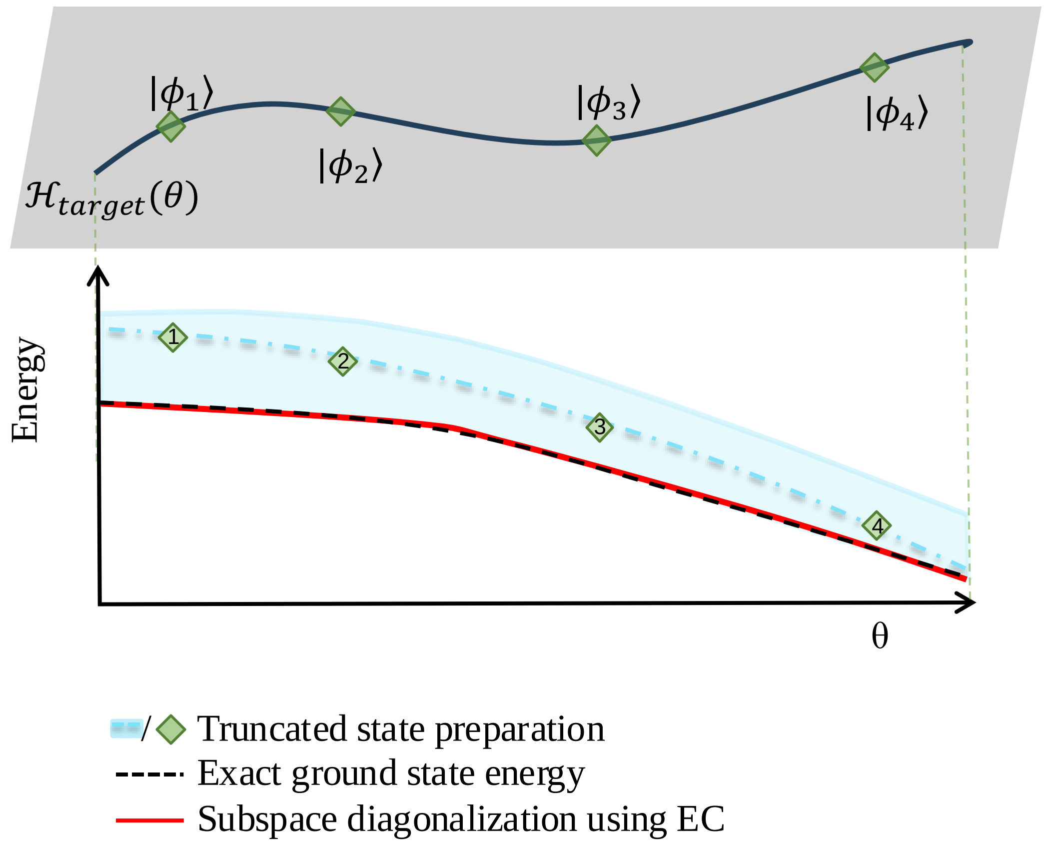
<u>Subspace Diagonalization using Eigenvector continuation</u>

Subspace $= \{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, |\phi_4\rangle\}$ ; $k_p = 4$ (in fig.)

$$\mathbb{H}(\theta)_{ij} = \langle \phi_i | H(\theta) | \phi_j \rangle$$

$$\mathbb{S}_{ij} = \langle \phi_i | \phi_j \rangle$$

$$\mathbb{H}(\theta)|\psi\rangle = E\,\mathbb{S}|\psi\rangle$$

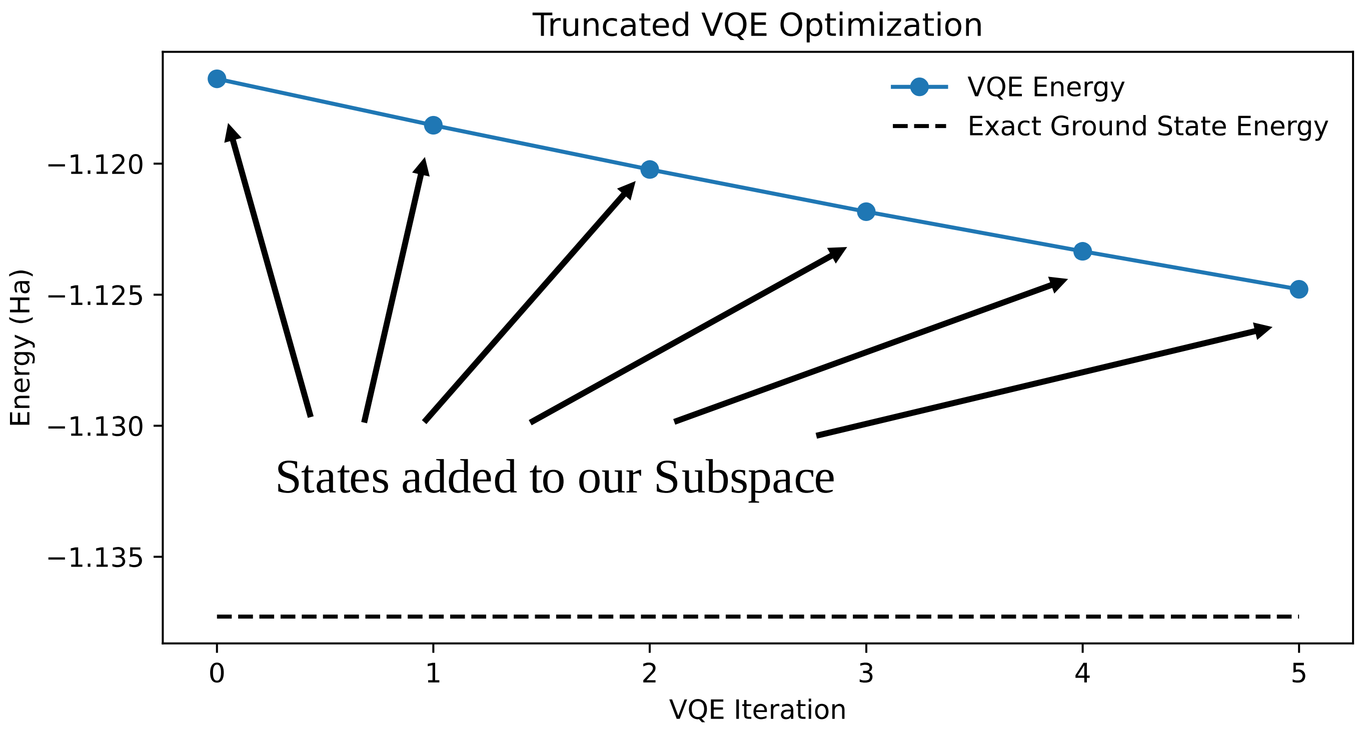


# Truncated VQE as our Basis

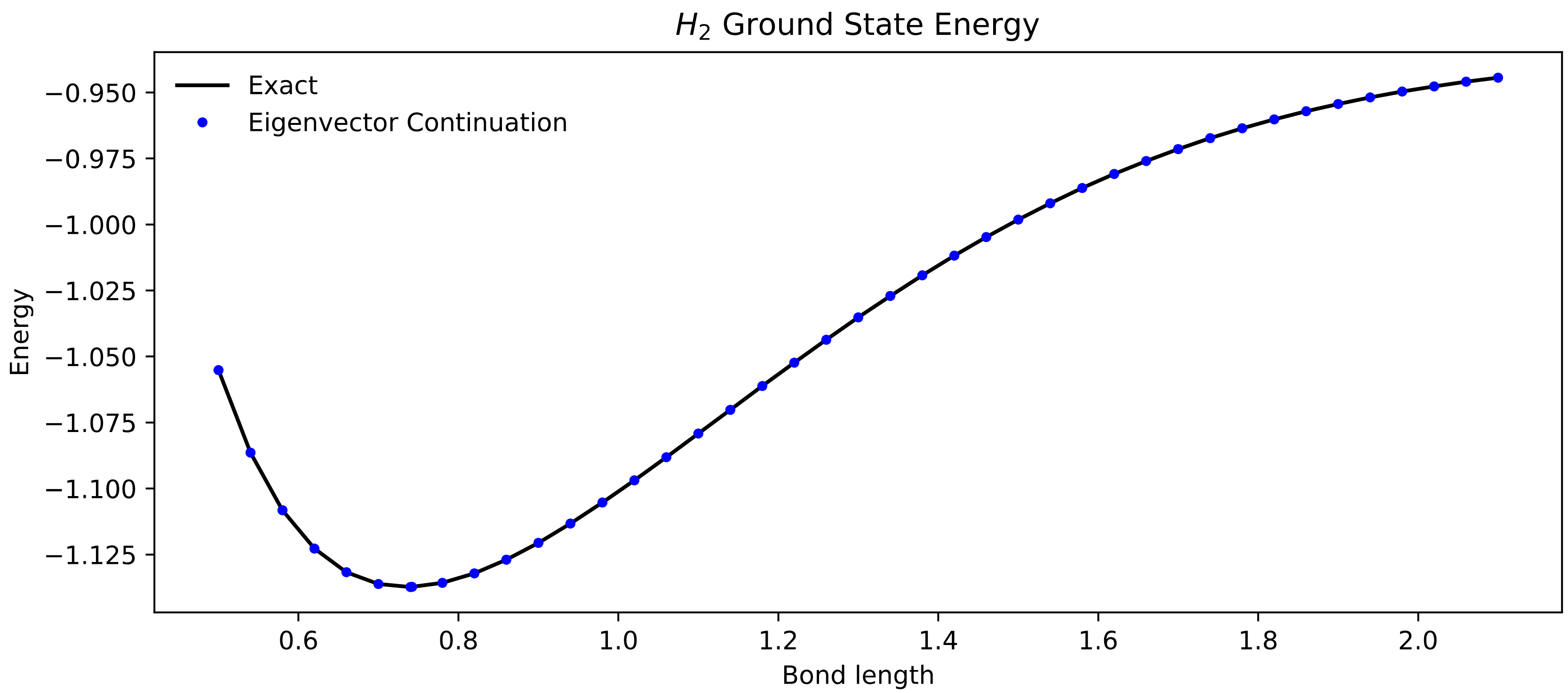
- Used UCCSD ansatz (60 CNOTS)

- Need only a few iterations of VQE for a subspace

- Employed a filtering procedure to ensure the subspace diagonalization is numerically stable
    1. Find the lowest energy state in subspace
    2. Add states with the least overlap to subspace – ensure the condition number is not too high
    3. Convergence is met when adding states doesn't change energy

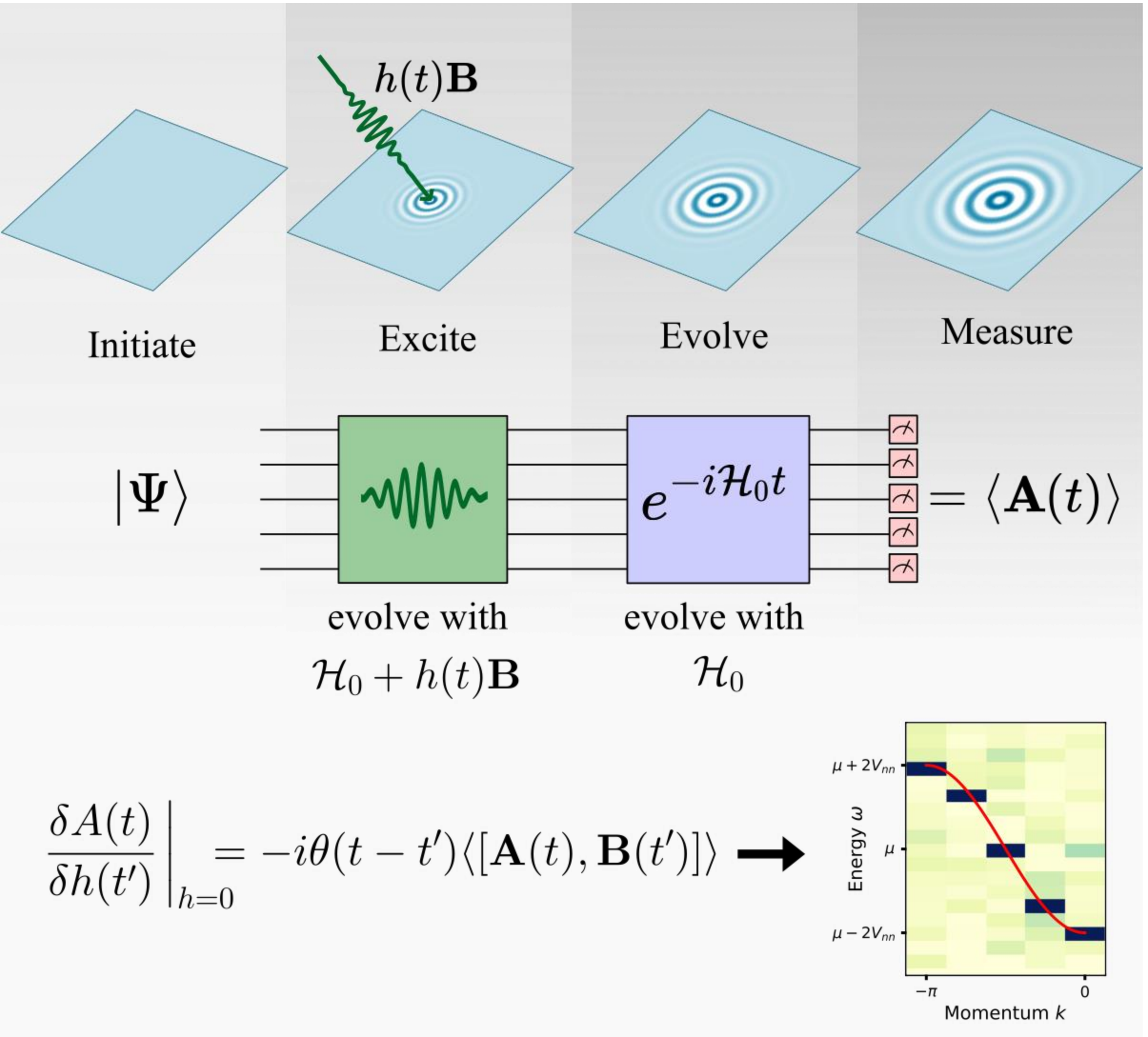


# H2 molecule spectrum using EC




- Only 2-4 states needed per data point
- VQE only done for 5 iterations with bond length of 0.74 A, but we get the *entire* spectrum!

# Linear Response and Quantum Simulations




Spectral Functions to measure energy differences $\epsilon_{nm}$ :

$$A_{jj}(T,\omega) = -\frac{1}{\pi} Im\ G^R_{jj}(\omega)$$

$$A_{jj}(T,\omega) = \bar{A}_{jj}(\omega) + R_{jj}(T,\omega),$$

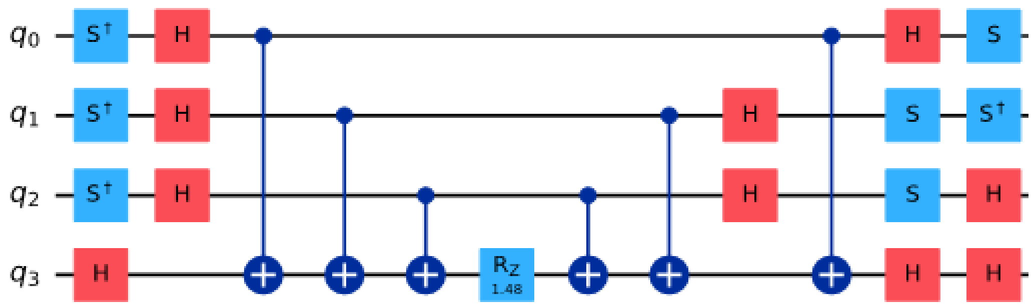
$$\bar{A}_{jj}(\omega) = \sum_{n,m} |\psi_n|^2 \left\{ \left|C^{(j)}_{nm}\right|^2 \delta(\omega - \epsilon_{nm}) + n \leftrightarrow m \right\},$$

Starting with the ground state we get from VQE+EC: we confine ourselves with peaks $\epsilon_{n0}$.

A way to get spectral gaps!

# Time evolution using Cartan decomposition

We used a fixed depth technique to simulate the time evolution operator. $U(t) = e^{-it\mathcal{H}}$

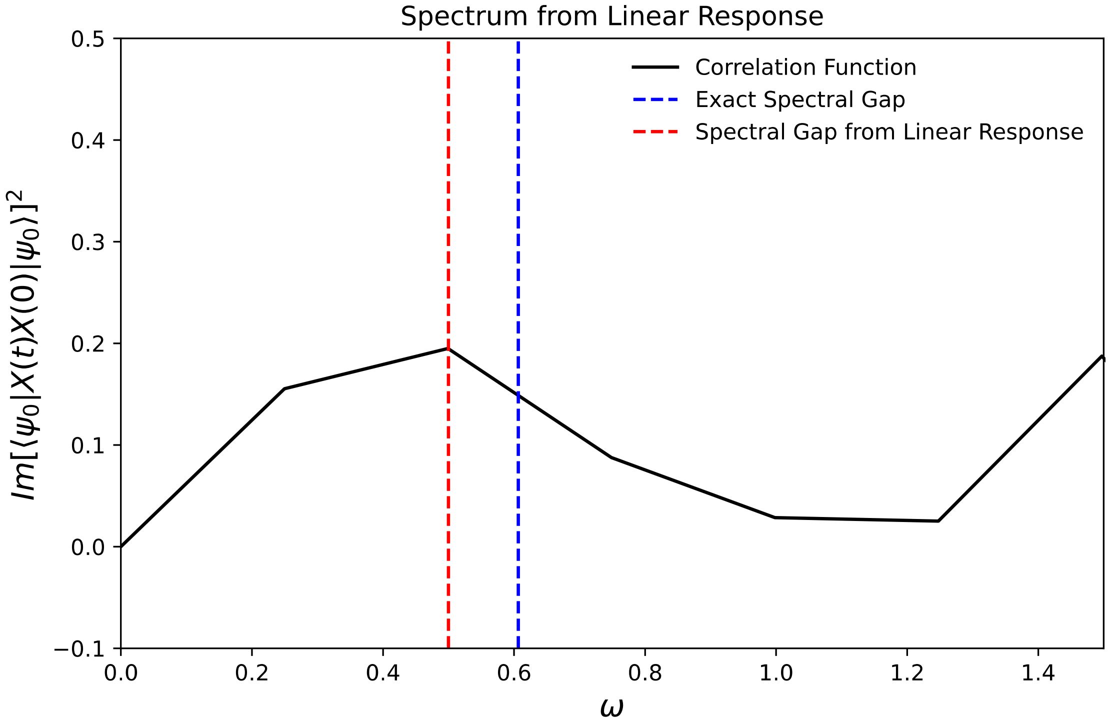



To compare:

- Direct circuit implementation (124 CNOTs)
- One first order Trotter step is (34 CNOTs)

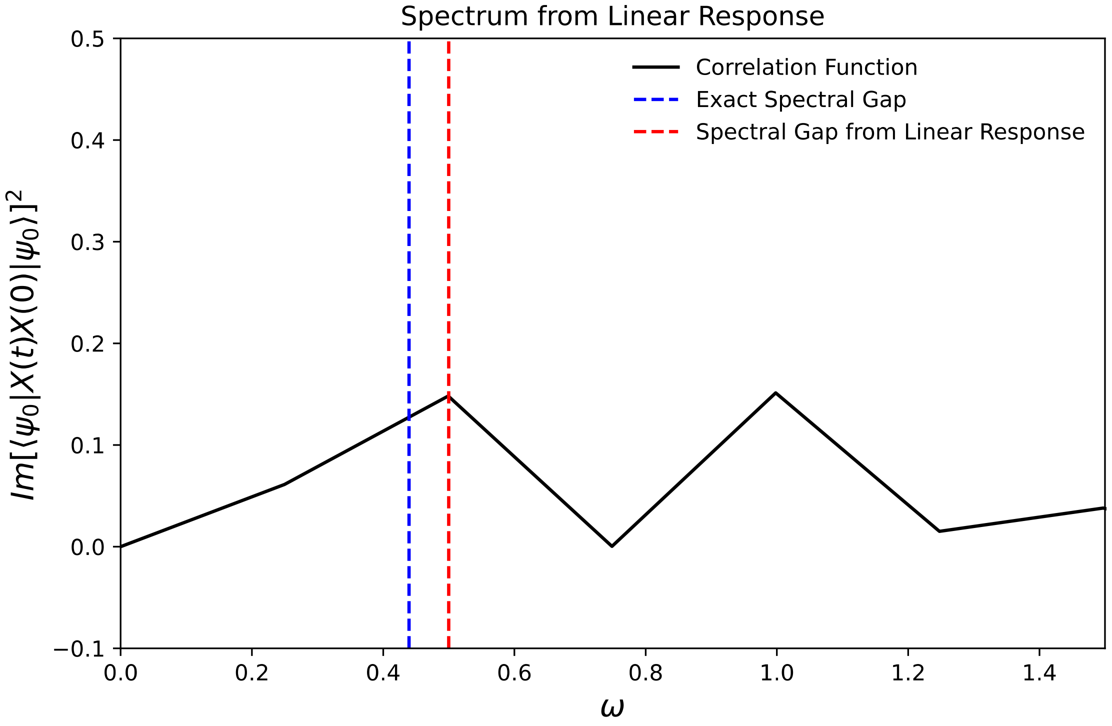
# Spectral gaps using Linear Response

Bond length = 0.74 A




Error: 17%

Bond length = 1.1 A




Error: 13%

# Conclusion

Right now:

VQE ➡ Eigenvector Continuation ➡ Cartan Fixed-Depth ➡ Linear Response

Next steps:

- Better VQE Ansatz
- Use Cartan for Imaginary Time Evolution to get excited states
- Post-processing signals
- Investigate other molecules

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# References


Eigenvector continuation:
1. Francis, Akhil, *et. al.*, 2209.10571
2. Agrawal, Anjali, *et. Al.*, 2406.17037
3. D. Frame *et. al.*, Phys. Rev. Lett. 121, 032501

Linear Response
1. Kökcü, E., *et. al.*, *Nat Commun* **15**, 3881 (2024)
2. Weidinger, Simon A., *et. Al.*, PhysRevB.98.224205

Cartan decomposition
1. Kökcü, E., *et. al.*, 2104.00728

Metallification of H2 molecule
1. Tiwary, P., *et. al.*, 10.1073/PNAS.1600917113
2. Bing, Li, *et, al.*, Phys. Rev. Lett. 126.036402

Resources
1. Pennylane (& their Quantum Chemistry Datasets)
2. QBraid
3. DoraHacks


Thank you!

# Paving the Way to science Experiments

## How do we know what electrons do inside matter?

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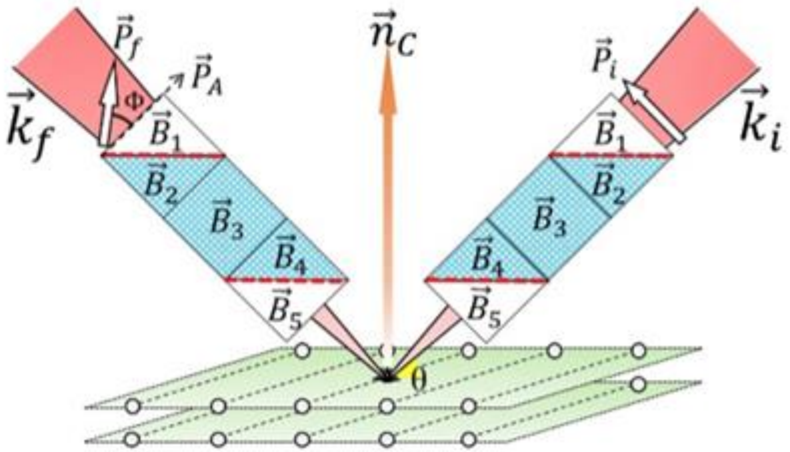
Neutron Scattering




Spin-Spin Correlations

Figure Courtesy Shen Group

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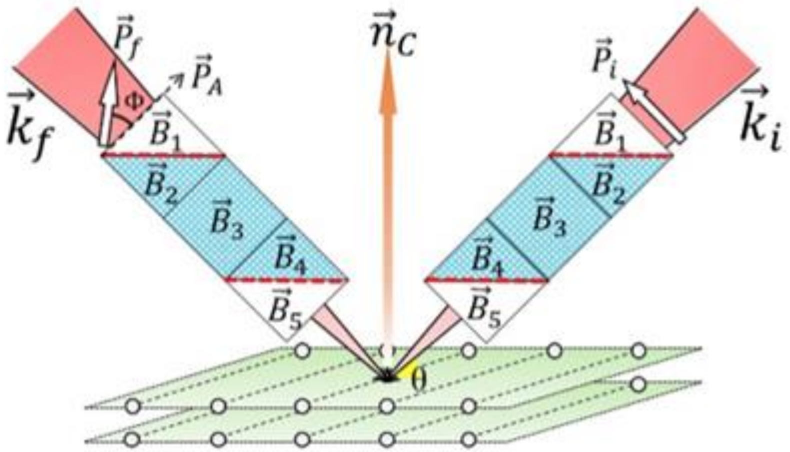


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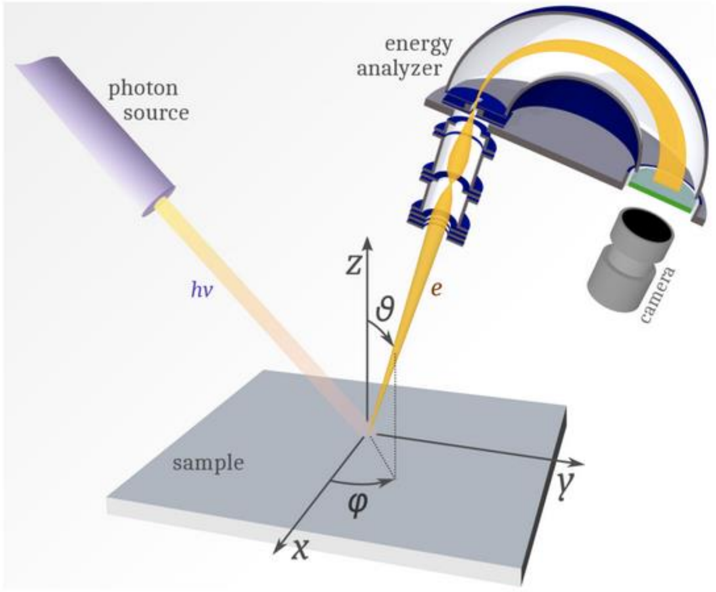
## Angle-Resolved Photoemission Spectroscopy




Single-Particle Green Functions

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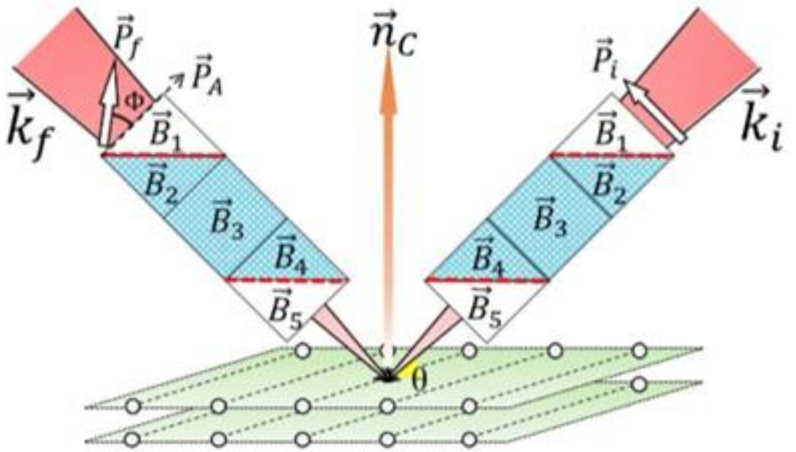


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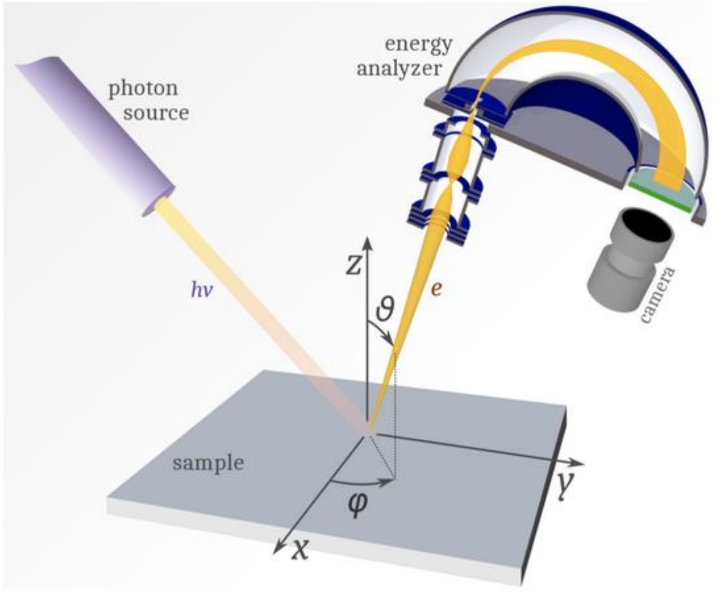


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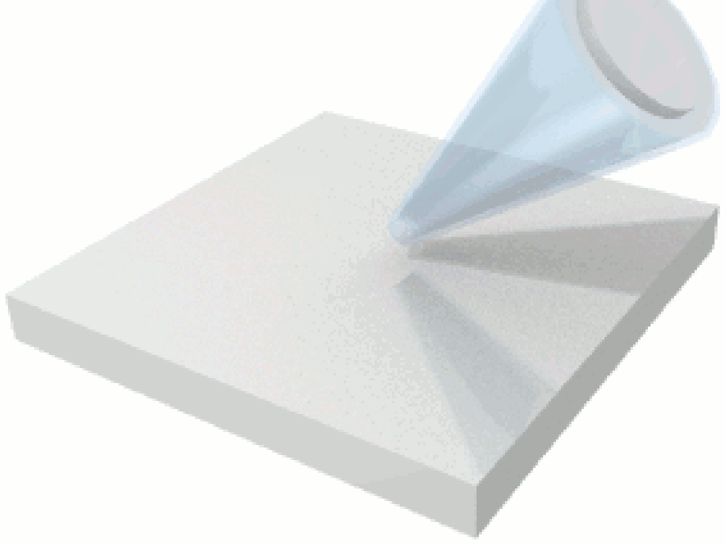
## Time-Resolved Photoemission Spectroscopy



Determining Band Structure

Animation courtesy [F. Schmitt](F. Schmitt)

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Consider: $H_0 = \sigma^z, A = B = \sigma^x$, A two-level system with $\Delta E = 2$:

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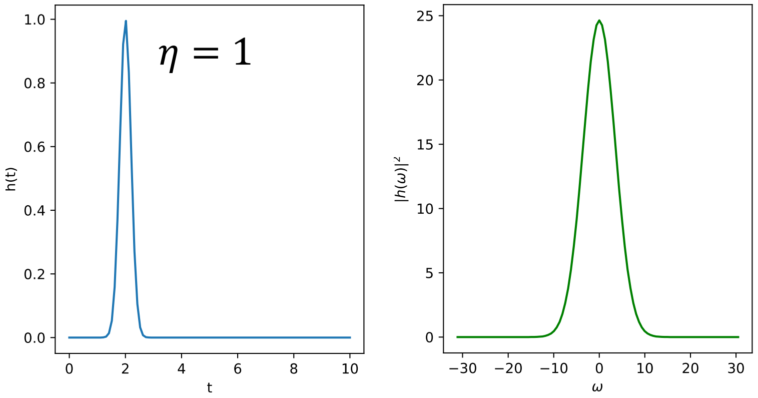

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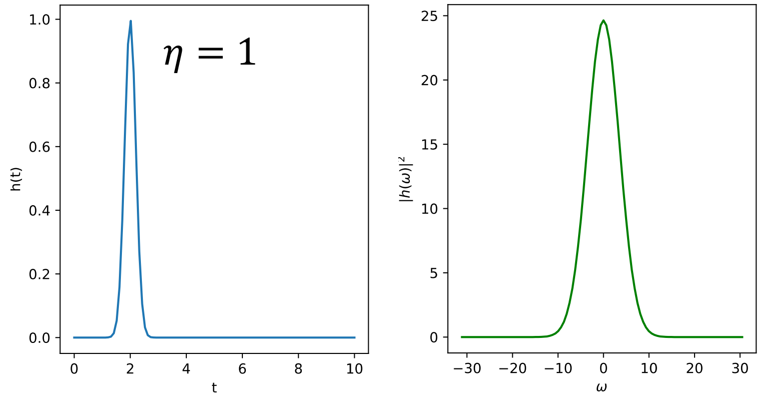


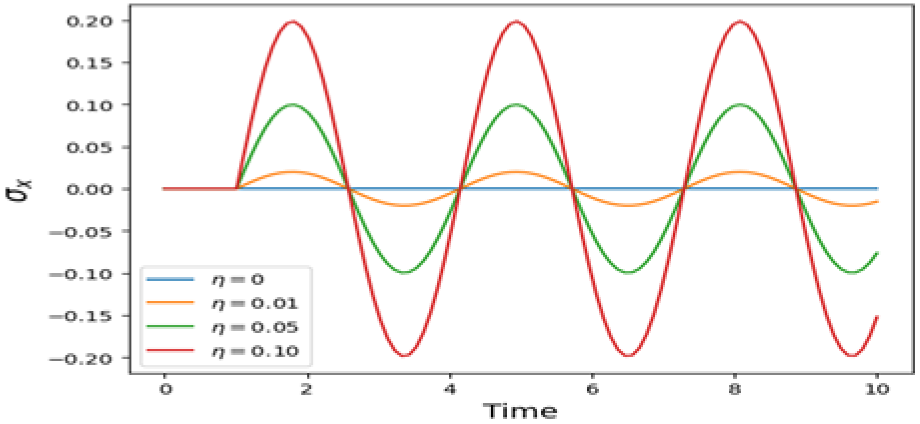

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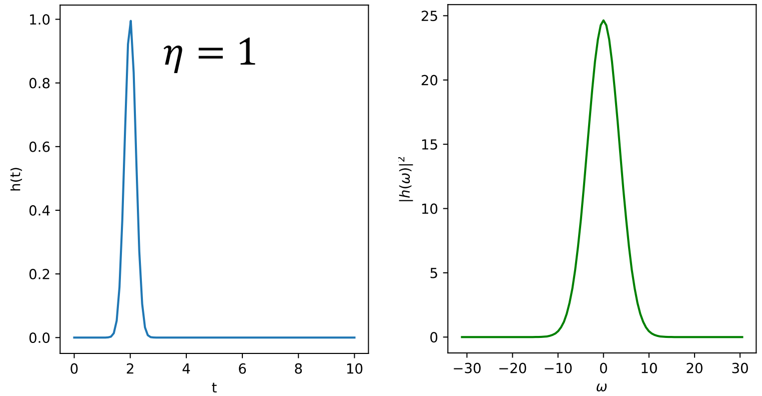


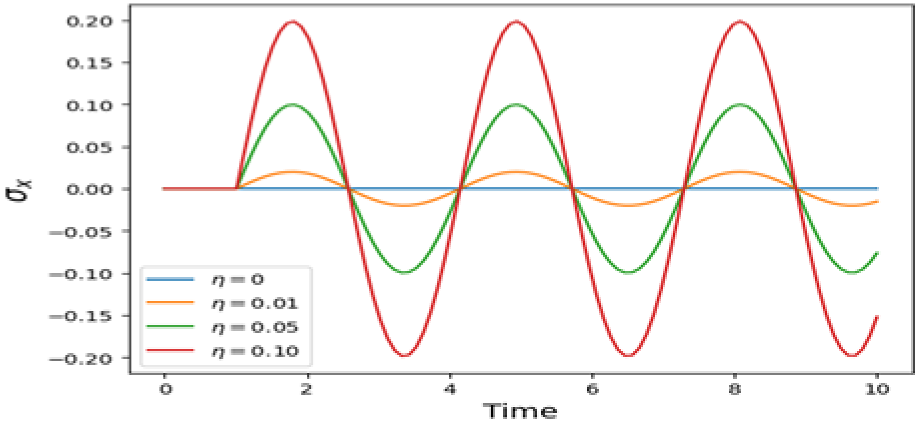


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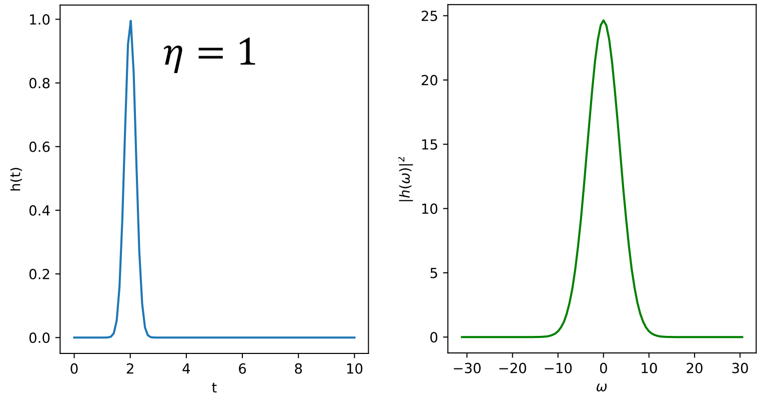


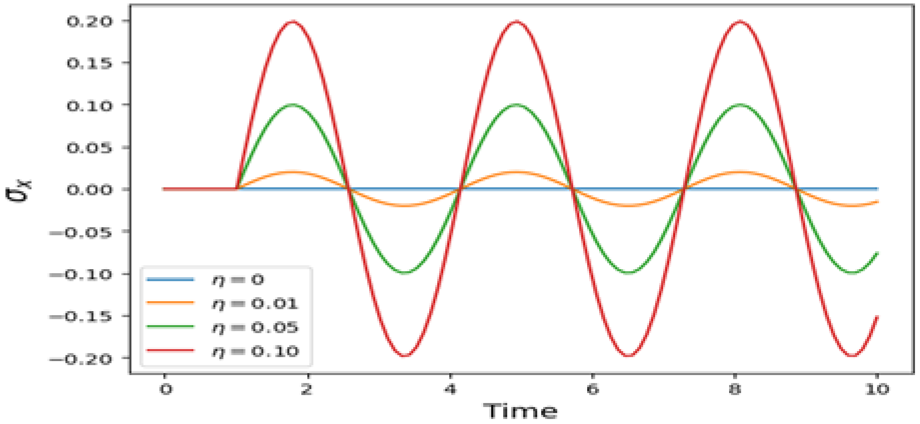


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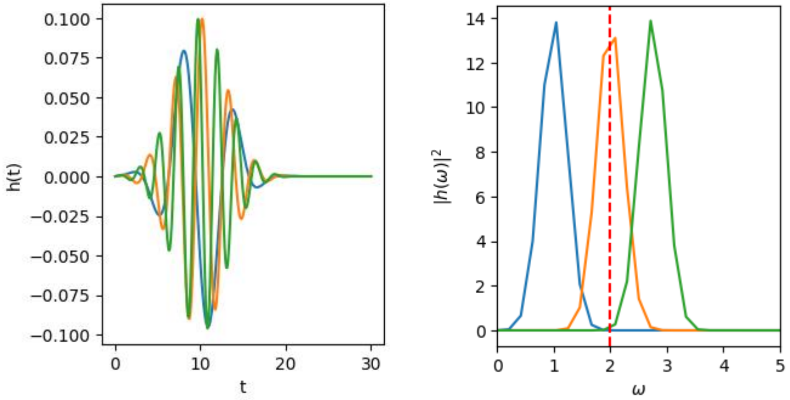

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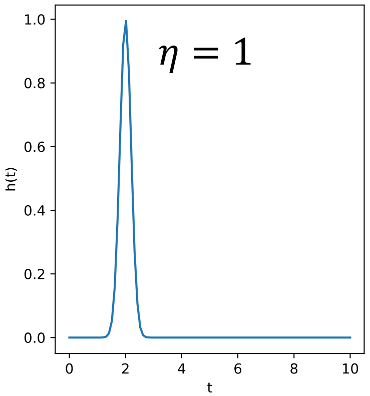


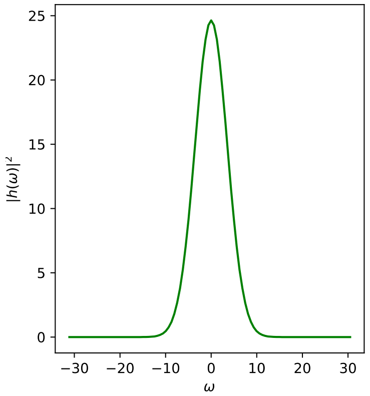


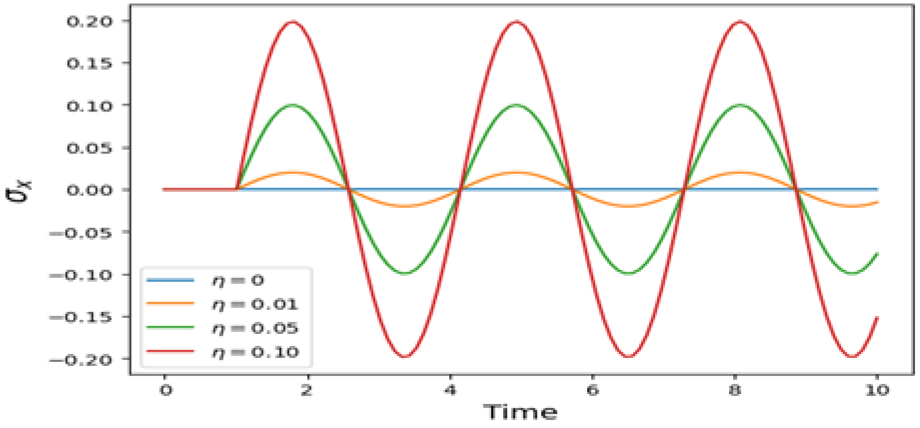


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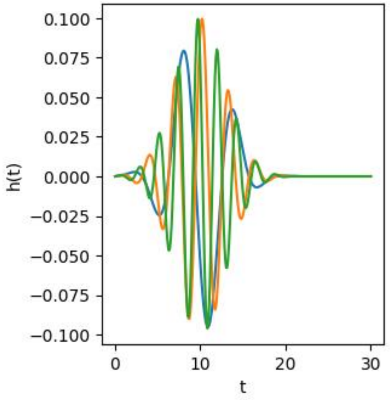


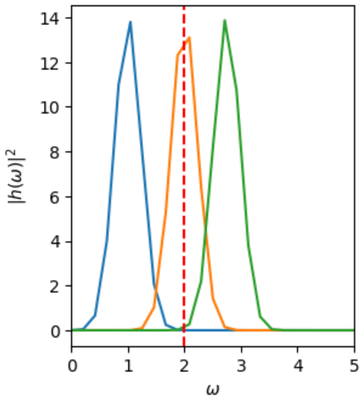


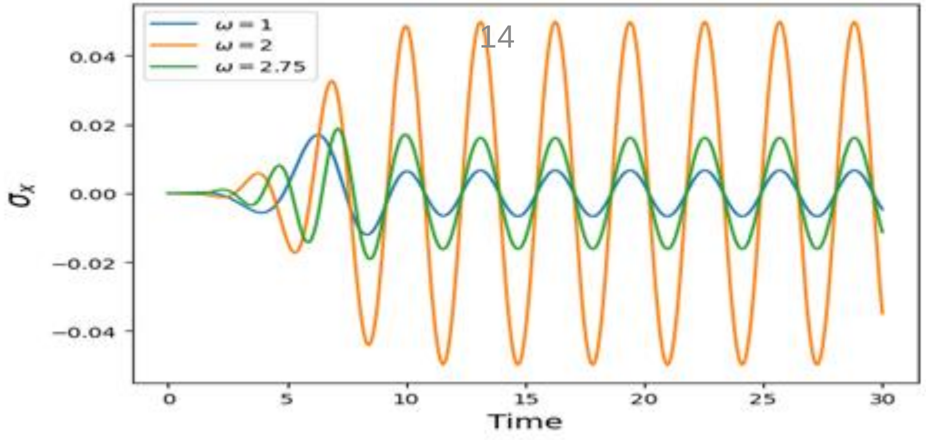

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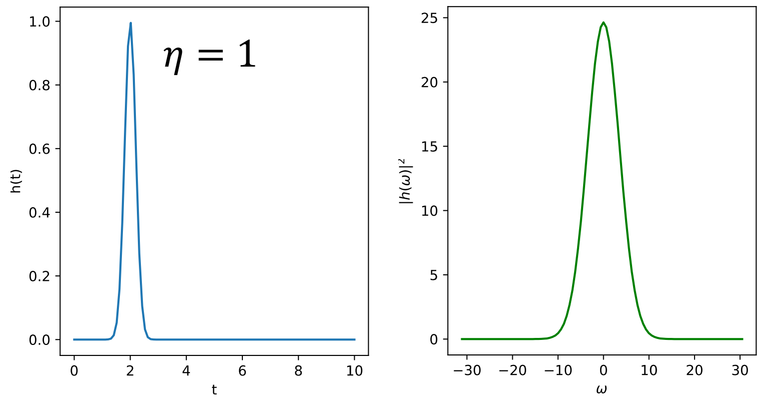


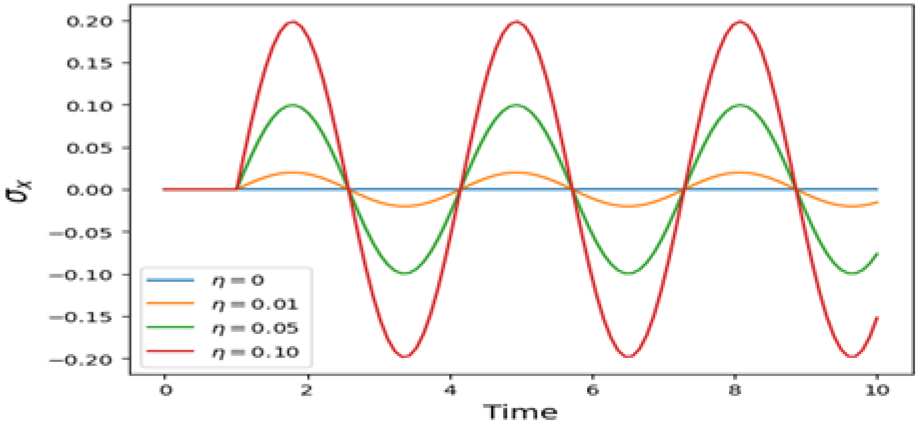


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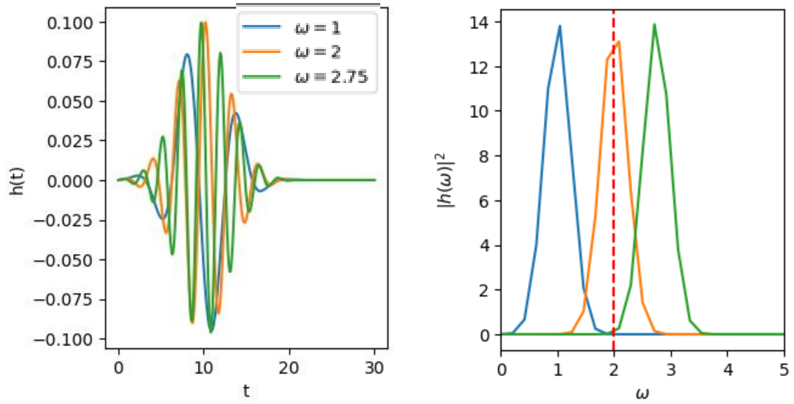


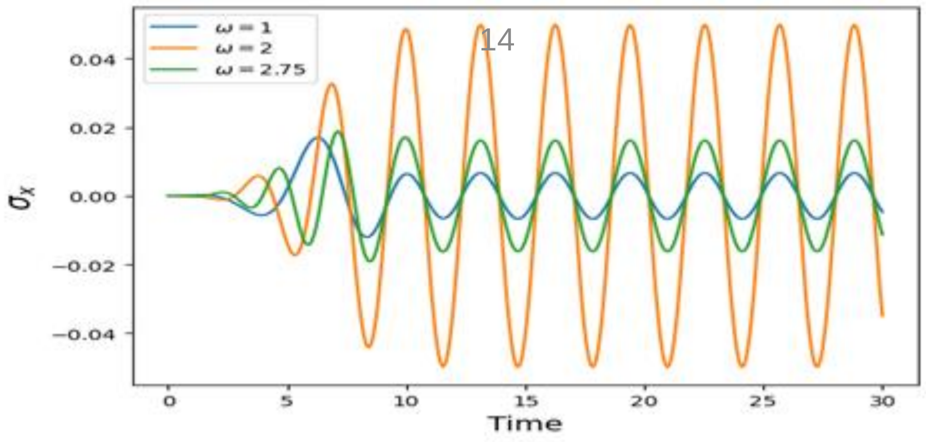

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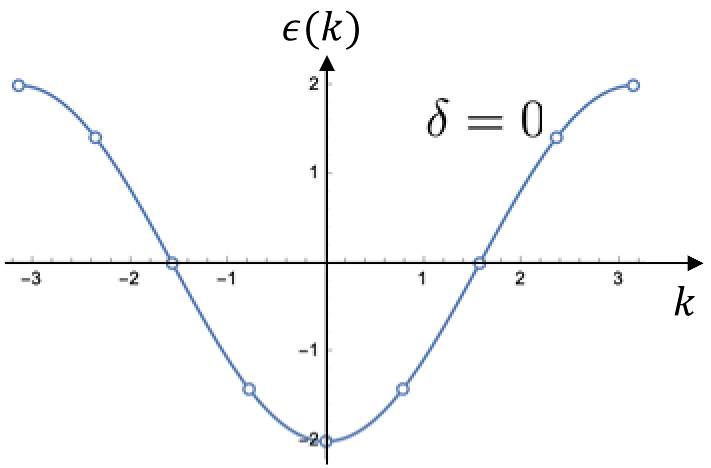

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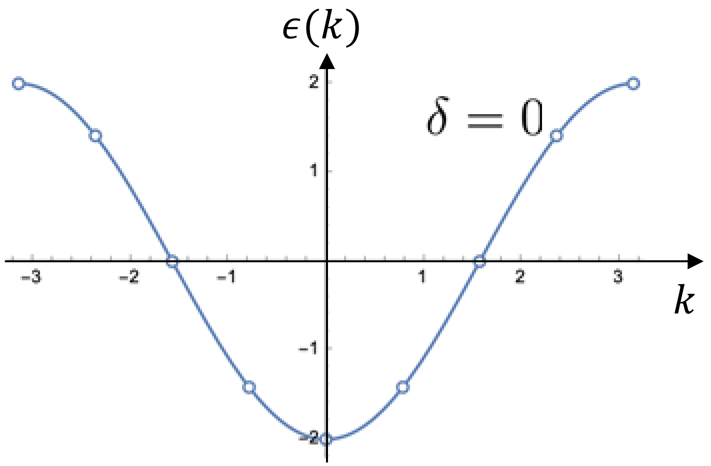


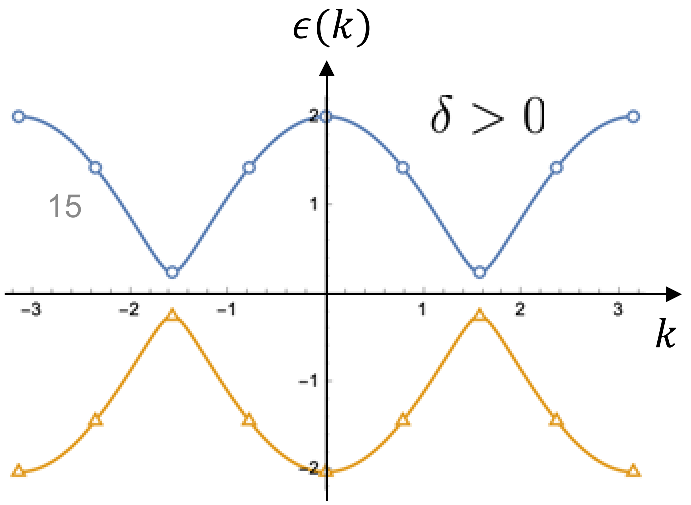

# Fermionic Correlation Functions

$$G^R(r_i,t;r_j,t') = -i\theta(t-t')\,\langle\psi_0|\{c_i(t),c_j^\dagger(t')\}|\psi_0\rangle$$

$$\mathbf{B} = \sum_i 2\cos(kr_i)\left[c_i + c_i^\dagger\right]$$

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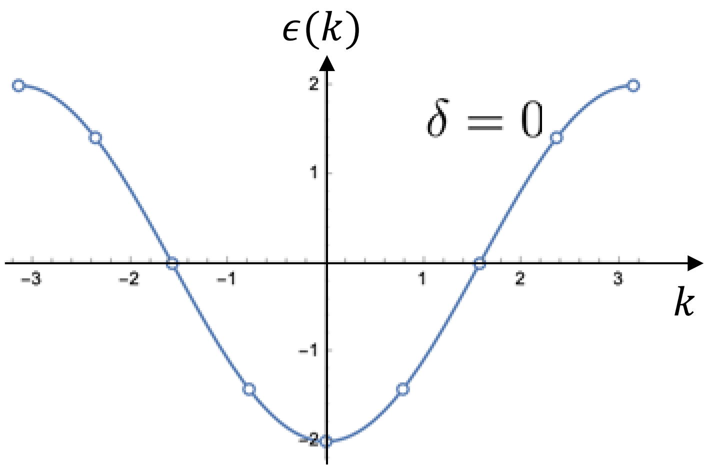


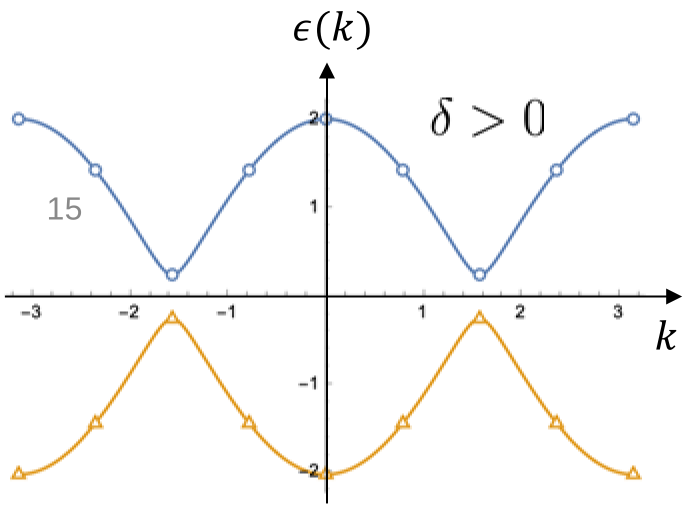


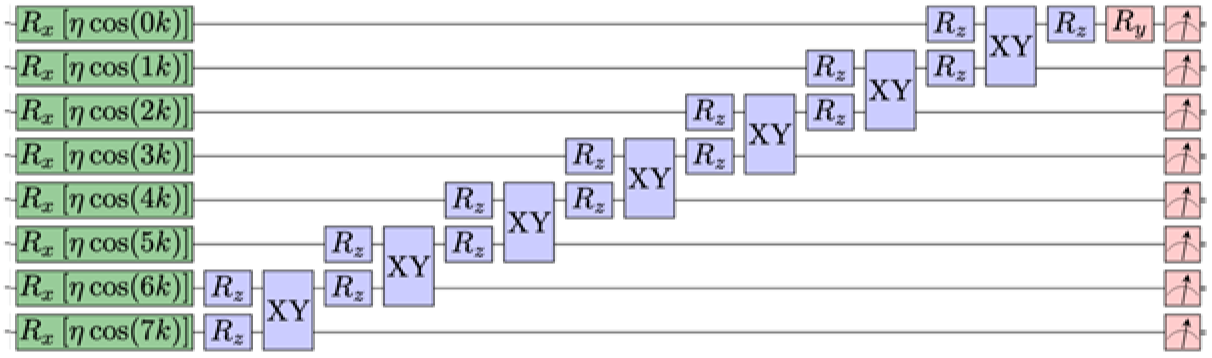


Compressed Circuit[] run *on ibm_auckland*

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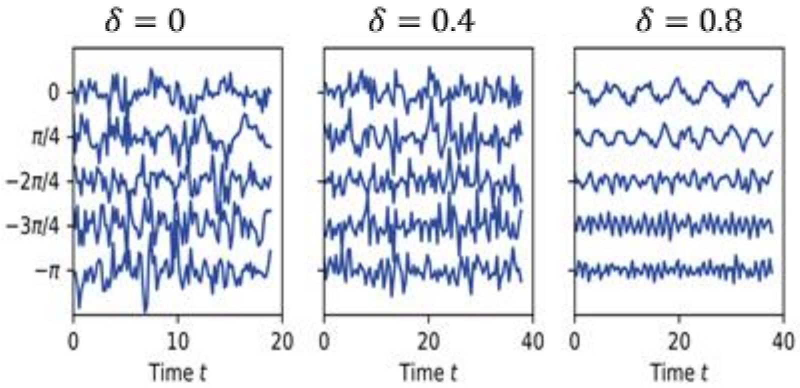


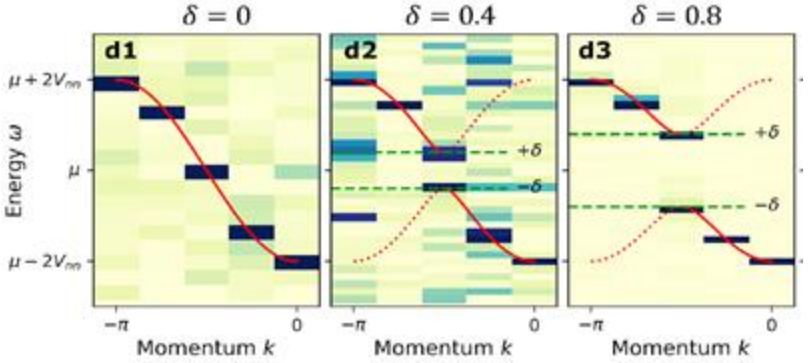


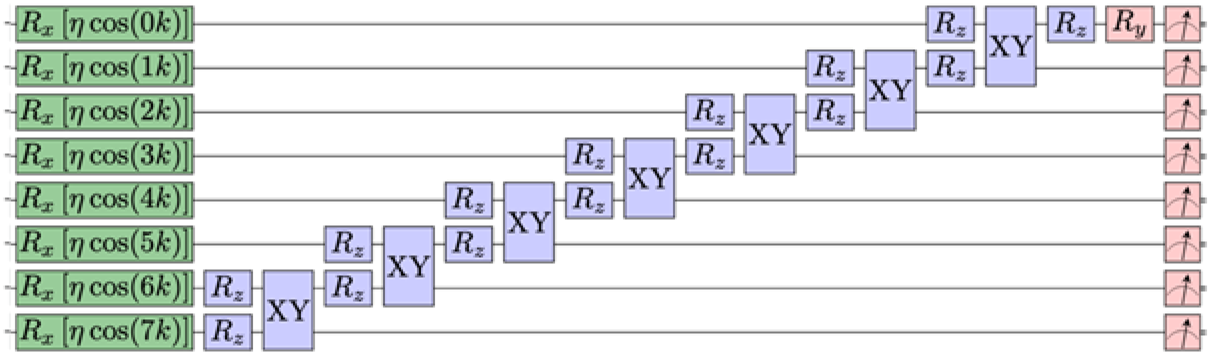


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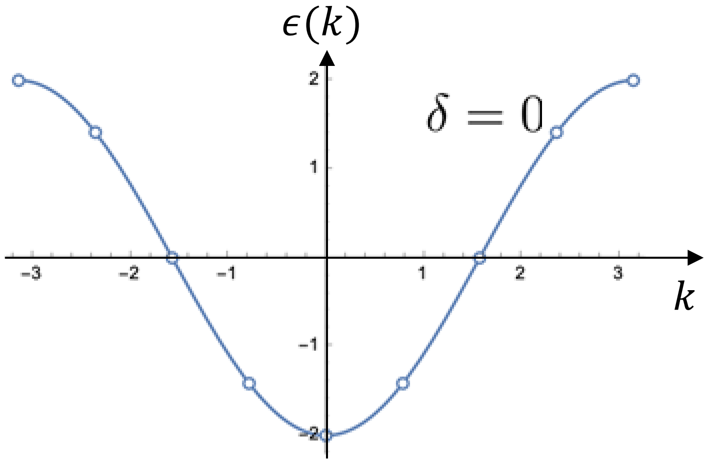


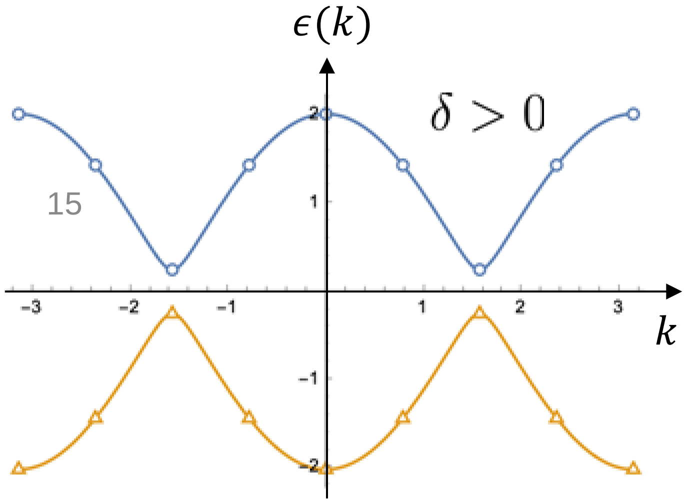

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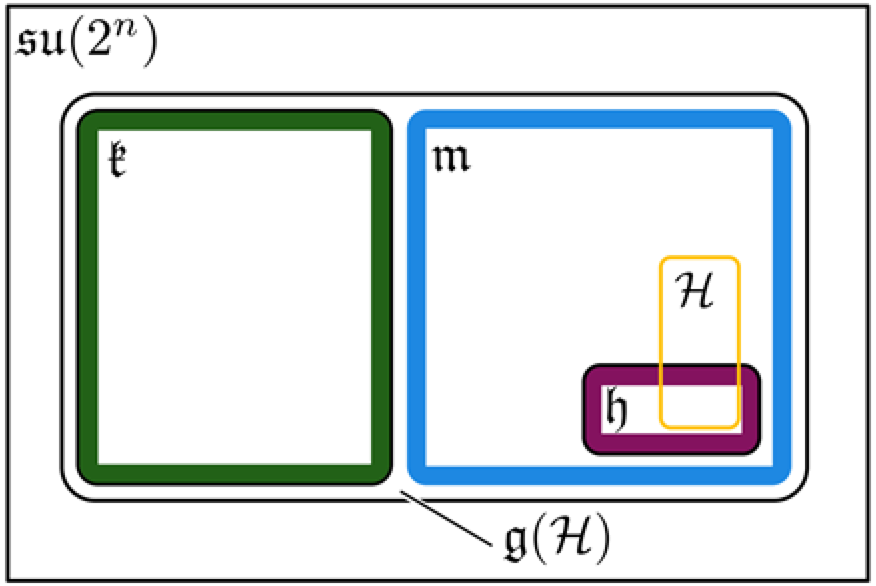
# Cartan Decomposition and KHK Theorem

**Definition 1** *Consider a compact semi-simple Lie subgroup* $G \subset SU(2^n)$, *which has a corresponding Lie subalgebra* $\mathfrak{g}$. *A* ***Cartan decomposition*** *on* $\mathfrak{g}$ *is defined as an orthogonal split* $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{m}$ *satisfying*

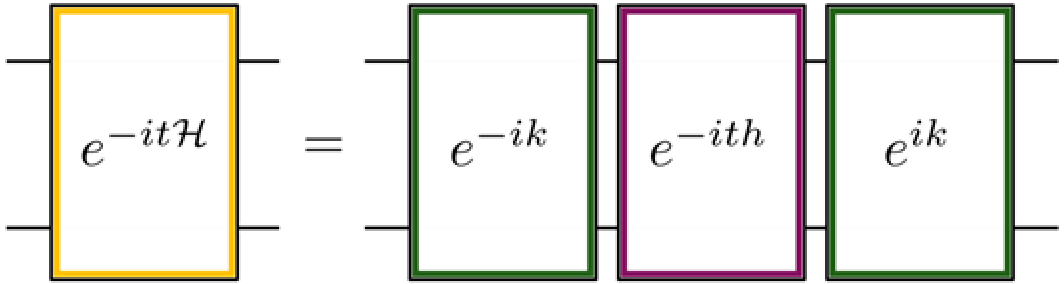
$$[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k} \qquad [\mathfrak{m}, \mathfrak{m}] \subset \mathfrak{k} \qquad [\mathfrak{k}, \mathfrak{m}] = \mathfrak{m} \tag{4}$$

*and is referred as* $(\mathfrak{g}, \mathfrak{k})$. ***Cartan subalgebra*** *of this decomposition is defined as one of the maximal Abelian subalgebras of* $\mathfrak{m}$, *and denoted as* $\mathfrak{h}$.

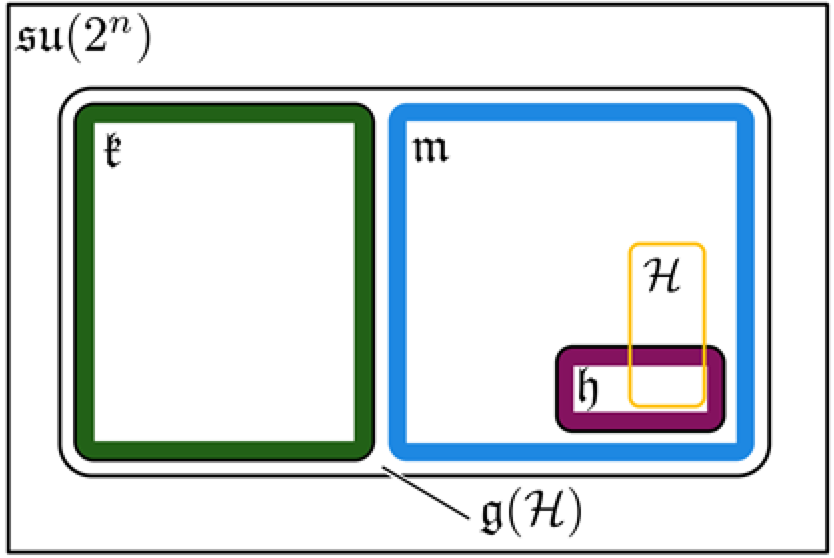



**Theorem 1** *Given a Cartan decomposition* $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{m}$, *for any element* $\mathcal{H} \in \mathfrak{m}$ *there exist a* $K \in e^{\mathfrak{k}}$ *and* $h \in \mathfrak{h}$ *such that*

$$\mathcal{H} = KhK^{\dagger} \tag{5}$$

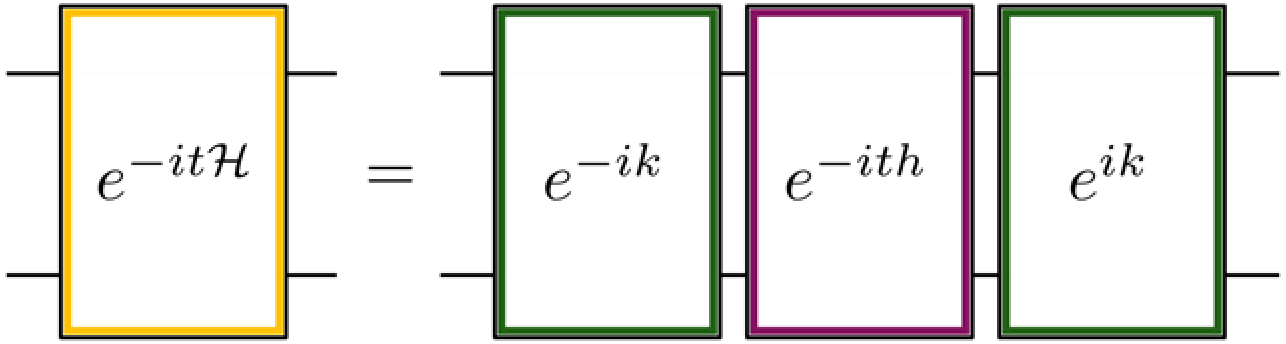


# Algorithm

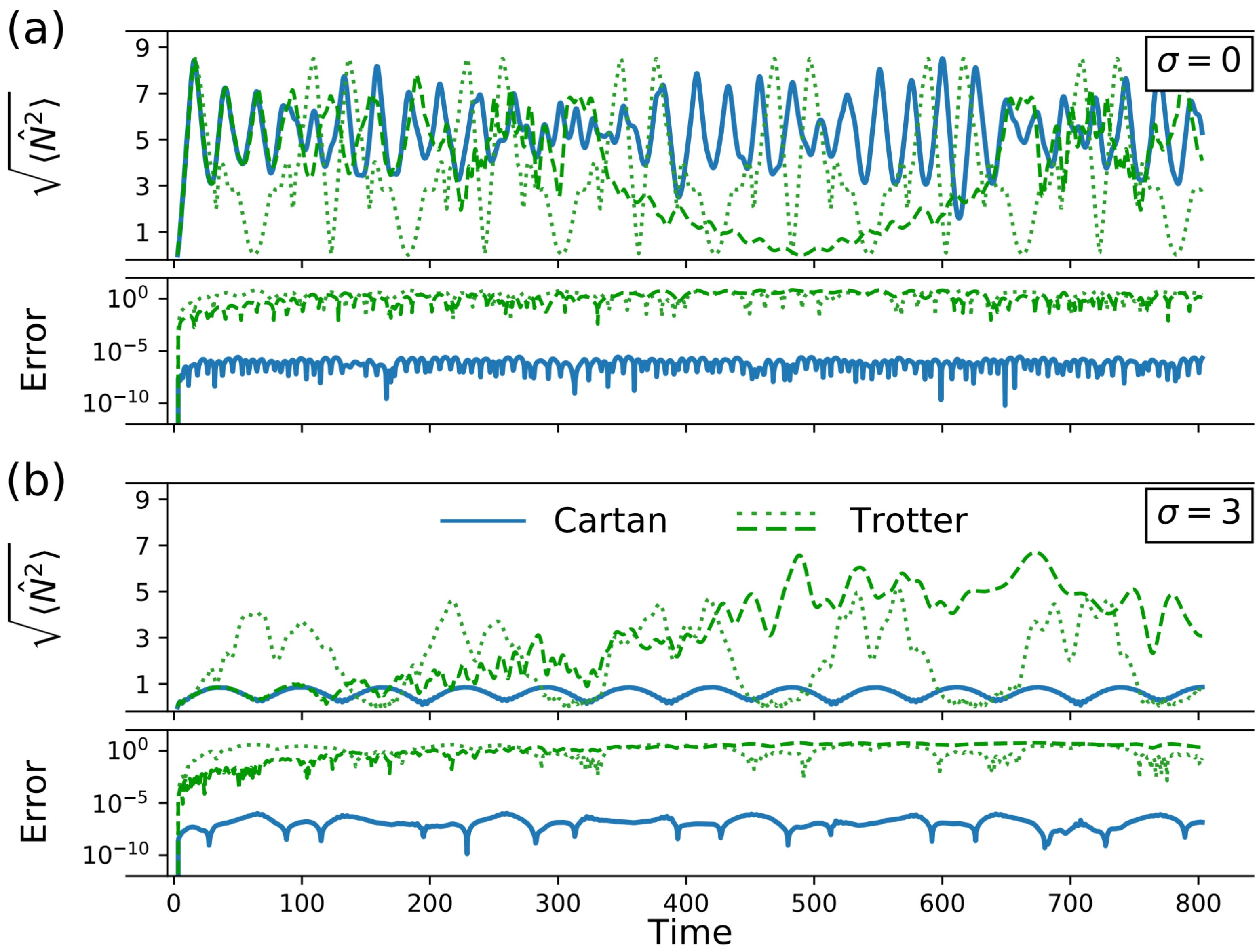



1) Generate Hamiltonian algebra g(H)
2) Find a Cartan decomposition such that H is in m
3) Fit parameters via minimizing f(K)
4) Build the circuit using K and h
5) Then simulate for any time you want!

$$f(K) = \langle KvK^{\dagger}, \mathcal{H} \rangle$$



# Results



(a)
$\sqrt{\langle \hat{N}^2 \rangle}$
9
7
5
3
1
$\sigma = 0$
Error
$10^0$
$10^{-5}$
$10^{-10}$
(b)
$\sqrt{\langle \hat{N}^2 \rangle}$
Cartan
Trotter
$\sigma = 3$
9
7
5
3
1
Error
$10^0$
$10^{-5}$
$10^{-10}$
0
100
200
300
400
500
600
700
800
Time